98333

Access DB# _____

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: FRANCISCO PRATS Examiner #: 71618 Date: 7-8-03
Art Unit: 1651 Phone Number 308-3665 Serial Number: 09/921,188
Mail Box and Bldg/Room Location: CM1-11A07 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: PROCESS FOR THE PREPARATIONS OF CHIRAL ISOFLUORENES

Inventors (please provide full names): JOHN F. CHIARELLO, BRIAN LEE BUCKWALTER, TIMOTHY CLAUDE BARDE

Earliest Priority Filing Date: 8-3-20

***For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.**

PLEASE SEARCH CLAIMS 10 AND 11 ATTACHED.

THANKS.

****

STAFF USE ONLY

Searcher: ~~Point of Contact:~~
Searcher Phone #: Alexandra Waclawiw
Searcher Location: ~~Technical Info. Specialist~~ CM1 6A02 Tel: 308-4491
Date Searcher Picked Up: 7-10-03
Date Completed: 7-10-03
Searcher Prep & Review Time: ~~30~~ 13
Clerical Prep Time: _____
Online Time: 28

Type of Search

NA Sequence (#) _____
AA Sequence (#) _____
Structure (#) 1
Bibliographic _____
Litigation _____
Fulltext _____
Patent Family _____
Other _____

Vendors and cost where applicable

STN $ 23500
Dialog _____
Questel/Orbit _____
Dr.Link _____
Lexis/Nexis _____
Sequence Systems _____
WWW/Internet _____
Other (specify) _____

DUP 10 1 2 28

PTO-1590 (1-2000)

STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 98333

TO: Frank Prats **Location: CM1/11A07/11B01** **Art Unit: 1651** **Thursday, July 10, 2003** **Case Serial Number: 921188**	**From: Alex Waclawiw** **Location: Biotech-Chem Library** **CM1-6A02** **Phone: 308-4491** **Alexandra.waclawiw@uspto.gov**

Search Notes

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     (FILE 'HCAPLUS' ENTERED AT 08:52:17 ON 10 JUL 2003)
               DEL HIS Y

     FILE 'REGISTRY' ENTERED AT 08:52:29 ON 10 JUL 2003
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L3          24 S L2 AND (CAPLUS OR CA)/LC
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:     8 JUL 2003  HIGHEST RN 544651-49-2
DICTIONARY FILE UPDATES:    8 JUL 2003  HIGHEST RN 544651-49-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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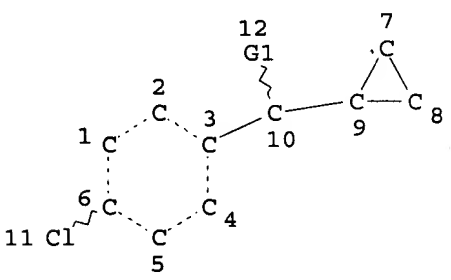

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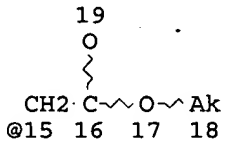

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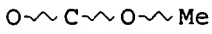

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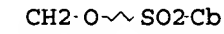

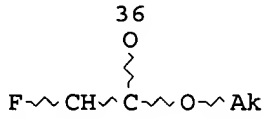


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  37

STEREO ATTRIBUTES: NONE
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FILE COVERS 1907 - 10 Jul 2003  VOL 139 ISS 2
FILE LAST UPDATED: 9 Jul 2003  (20030709/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

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L5           12 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L2


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L5   ANSWER 1 OF 12  HCAPLUS  COPYRIGHT 2003 ACS
ACCESSION NUMBER:         2002:122926  HCAPLUS
DOCUMENT NUMBER:          136:183615
TITLE:                    Process for the preparation of chiral insecticidal and
                          acaricidal 1,4-diaryl-2-fluoro-2-butenes via enzymic
                          hydrolysis of (4-chlorophenyl)cyclopropylethanoic acid
                          methyl ester using esterase
INVENTOR(S):              Chiarello, John Francis; Buckwalter, Brian Lee;
                          Barden, Timothy Claude
PATENT ASSIGNEE(S):       Basf Aktiengesellschaft, Germany
SOURCE:                   PCT Int. Appl., 75 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND  DATE           APPLICATION NO.  DATE
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     WO 2002012155        A2   20020214       WO 2001-EP9012   20010803
     WO 2002012155        A3   20021128
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
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LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,
RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ,
VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2002032351	A1	20020314	US 2001-921188	20010802
AU 2001082067	A5	20020218	AU 2001-82067	20010803
EP 1307418	A2	20030507	EP 2001-960622	20010803

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

PRIORITY APPLN. INFO.: US 2000-222733P P 20000803
WO 2001-EP9012 W 20010803

OTHER SOURCE(S): CASREACT 136:183615; MARPAT 136:183615

AB There is provided a process for the prepn. of a chiral compd. of formula ArC*H(R)CF:CHAr1 [I; Ar, Ar1 = (un)substituted aryl or a 5- or 6-membered heteroarom. ring; R is C1-4 alkyl, C1-4 haloalkyl, C3-6 cycloalkyl or C3-6 halocycloalkyl; Ar1 , is aryl or a 5- or 6-membered heteroarom. ring; C* represents an asym. center] which is useful as an insecticidal and acaricidal agent and for protecting plants from damage caused by insect and acarid attack and infestation (no data). Also provided are intermediate compds. useful in the process of the present invention. This process comprises (a) treating a racemic ester of formula ArCH(R)CO2R4 (II; Ar, R = same as above; R4 = C1-4 alkyl) with an esterase to form a first mixt. of either R-acid of formula ArCH(R)CO2H (III) and S-ester of formula II or of S-acid of formula III and R-ester of formula II, (b) sepg. (R)- or (S)-acid III from said (S)- or (R)-ester II, (c) reducing the chiral acid (R)- or (S)-acid III or (S)- or (R)-ester II to obtain a chiral alc. of formula (R)- or (S)-ArC*H(R)CH2OH, (d) transforming the chiral alc. into an ester (R)- or (S)-ArC*H(R)CH2CO2R1, (e) fluorinating the latter ester to afford a fluoro-ester (R)- or (S)-ArC*H(R)CHFCO2R1, and (f) reacting the latter fluoro-ester with an aldehyde Ar1CH2CHO (Ar1 = same as above) in a solvent in the presence of a base to afford a second mixt. of 4 chiral diastereomeric hydroxy-esters ArC*H(R)CHF(CO2R1)CH(OH)CH2Ar1. It further comprises (g) optionally sepg. the second mixt. into a third mixt. each having two chiral diastereomers, (h) treating the hydroxy-ester mixts. with an acylating agent R2COX1 (R2 = C1-4 alkyl; X1 = Cl, Br, R2CO2) to afford a fifth mixt. of 4 chiral diastereomeric acyloxy esters or a seventh mixt. of two chiral diastereomeric acyloxy esters ArC*H(R)CHF(CO2R1)CH(O2CR2)CH2Ar1, (i) optionally sepg. the sixth or seventh mixt. not essentially pure chiral diastereomeric acyloxy ester, (j) hydrolyzing the pure acyloxy esters or mixts. of esters to afford a hydroxy acid ArC*H(R)CHF(CO2H)CH(OH)CH2Ar1, and (k) heating the hydroxy acid with a arylsulfonyl halide to afford I. Thus, Me (2RS)-(4-chlorophenyl)(cyclopropyl)ethanoate was treated with horse liver esterase in water (pH 7.5) to give 37.9% (2R)-(4-chlorophenyl)(cyclopropyl)ethanoic acid and 36.2% Me (2S)-(4-chlorophenyl)(cyclopropyl)ethanoate, each of which was reduced by BH3.THF/THF at room temp. for 4 h and DIBAL/CH2Cl2 warming from -78.degree. to room temp. and at room temp. for 1 h, resp., to give 84% (2R)-(4-chlorophenyl)(cyclopropyl)ethanol and 80% (2S)-(4-chlorophenyl)(cyclopropyl)ethanol, resp. Each of (2R)- and (2S)-(4-chlorophenyl)(cyclopropyl)ethanol was tosylated by tosyl chloride in the presence of Et3N in CH2Cl2 to (2R)- and (2S)-(4-chlorophenyl)(cyclopropyl)ethyl p-toluenesulfonate, resp., which underwent cyanation with NaCN in DMSO at 90.degree. for 3 h to give (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropylpropanenitrile, resp. Alkali hydrolysis of (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropylpropanenitrile in a mixt. of 10% aq. NaOH and methanol under reflux for 18 h followed by acidification with concd. HCl gave (2R)- and

(2S)-3-(4-chlorophenyl)-3-cyclopropylpropanoic acid, resp., which was esterified with MeOH in the presence of HCl at room temp. for 18 h gave Me (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropylpropanoate, resp. Lithiation of the each ester with lithium diisopropylamide (LDA) in THF at -78.degree. to 0.degree. followed by fluorination with (PhSO2)2NF at -78.degree. to room temp. and room temp. for 2 h gave Me (2R)- and (2S)-3-(4-chlorophenyl)-3-cyclopropyl-2-fluoropropanoate, resp. Lithiation of Me (2S)-3-(4-chlorophenyl)-3-cyclopropyl-2-fluoropropanoate with LDA in THF at -78.degree. for 15 min followed by addn. reaction with 4-fluoro-3-phenoxyphenylacetaldehyde at -78.degree. for 2 h gave, after silica gel chromatog., an oil (A) contg. (2R,3R) and (2R,3S) or (2S,3R)-Me 2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoate and an oil contg. (2S,3S) and (2S,3R) or (2R,3S)-Me 2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoate (steps f and g). Acetylation of the oil A with Ac2O in the presence of DAMP in CH2Cl2 at room temp. for 2 h gave Me (2R,3R)-3-(acetyloxy)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate and Me (2R,3S or 2S,3R)-3-(acetyloxy)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate (step h and i). Alkali hydrolysis of the latter diastereomer in a mixt. of 10% aq. NaOH, MeOH, and THF under reflux for 1 h gave (2S,3R or 2R,3S)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoic acid (step j) which was heated with tosyl chloride in collidine at 170.degree. for 2 h to give 4-[(2Z,4S)-4-(4-chlorophenyl)-4-cyclopropyl-3-fluoro-2-butenyl]-1-fluoro-2-phenoxybenzene as a colorless oil (step k).

IC ICM C07C043-29
ICS C07C033-50; C07C057-62; C07C069-65; C07C069-736; C07C255-35; C07C309-73; C12P041-00

CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 5

IT **398453-51-5P**, (2R)-(4-Chlorophenyl)(cyclopropyl)ethanoic acid
398453-52-6P, Methyl (2S)-(4-chlorophenyl)(cyclopropyl)ethanoate
RL: BPN (Biosynthetic preparation); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; process for prepn. of chiral insecticidal and acaricidal diarylfluorobutenes via enzymic hydrolysis of (4-chlorophenyl)cyclopropylethanoic acid Me ester using esterase)

IT 68359-57-9P, 4-Fluoro-3-phenoxybenzaldehyde 117252-07-0P, 2-(4-Fluoro-3-phenoxyphenyl)acetaldehyde **119544-59-1P**, (2R)-2-(4-Chlorophenyl)-2-cyclopropylethanol **119544-60-4P**, (2S)-2-(4-Chlorophenyl)-2-cyclopropylethanol 398453-50-4P, 1-Fluoro-4-((E)-2-methoxyethenyl)-2-phenoxybenzene **398453-53-7P**, (2R)-2-(4-Chlorophenyl)-2-cyclopropylethyl 4-methylbenzenesulfonate **398453-54-8P**, (2S)-2-(4-Chlorophenyl)-2-cyclopropylethyl 4-methylbenzenesulfonate **398453-55-9P**, (3R)-3-(4-Chlorophenyl)-3-cyclopropylpropanenitrile **398453-56-0P**, (3S)-3-(4-Chlorophenyl)-3-cyclopropylpropanenitrile **398453-57-1P**, (3R)-3-(4-Chlorophenyl)-3-cyclopropylpropanoic acid **398453-58-2P**, (3S)-3-(4-Chlorophenyl)-3-cyclopropylpropanoic acid **398453-59-3P**, Methyl (3R)-3-(4-chlorophenyl)-3-cyclopropylpropanoate **398453-60-6P**, Methyl (3S)-3-(4-chlorophenyl)-3-cyclopropylpropanoate **398453-61-7P**, Methyl (3R)-3-(4-chlorophenyl)-3-cyclopropyl-2-fluoropropanoate **398453-62-8P**, Methyl (3S)-3-(4-chlorophenyl)-3-cyclopropyl-2-fluoropropanoate 398453-63-9P, Methyl (2R,3R)-3-(acetyloxy)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate 398453-64-0P, Methyl (2S,3S)-3-(acetyloxy)-2-

[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate 398453-66-2P, Methyl (2S,3S)-3-(acetyloxy)-2-[(R)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-2-phenoxyphenyl)butanoate 398453-67-3P, Methyl (2R,3R)-3-(acetyloxy)-2-[(R)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate 398453-68-4P, Methyl (2S,3S)-3-(acetyloxy)-2-[(R)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate 398453-69-5P, (2S,3S)-2-[(S)-(4-Chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoic acid 398453-70-8P, (2R,3R)-2-[(S)-(4-Chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoic acid 398453-71-9P, (2R,3R)-2-[(R)-(4-Chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-3-hydroxybutanoic acid 398453-76-4P 398453-77-5P, Methyl (2R,3S)-3-(acetyloxy)-2-[(S)-(4-chlorophenyl)(cyclopropyl)methyl]-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)butanoate 398453-78-6P 398453-79-7P 398453-80-0P 398453-81-1P 398453-82-2P 398453-83-3P 398453-84-4P 398464-67-0P 398464-69-2P 398464-70-5P 398464-71-6P 398464-73-8P 398464-74-9P 398464-75-0P 398464-76-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; process for prepn. of chiral insecticidal and acaricidal diarylfluorobutenes via enzymic hydrolysis of (4-chlorophenyl)cyclopropylethanoic acid Me ester using esterase)

IT 108-24-7, Acetic anhydride 4009-98-7, (Methoxymethyl)triphenylphosphonium chloride 68359-55-7, 4-(Bromomethyl)-1-fluoro-2-phenoxybenzene **119544-56-8**, Methyl (2RS)-(4-chlorophenyl)(cyclopropyl)ethanoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; process for prepn. of chiral insecticidal and acaricidal diarylfluorobutenes via enzymic hydrolysis of (4-chlorophenyl)cyclopropylethanoic acid Me ester using esterase)

IT **398453-51-5P**, (2R)-(4-Chlorophenyl)(cyclopropyl)ethanoic acid **398453-52-6P**, Methyl (2S)-(4-chlorophenyl)(cyclopropyl)ethanoate
RL: BPN (Biosynthetic preparation); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; process for prepn. of chiral insecticidal and acaricidal diarylfluorobutenes via enzymic hydrolysis of (4-chlorophenyl)cyclopropylethanoic acid Me ester using esterase)

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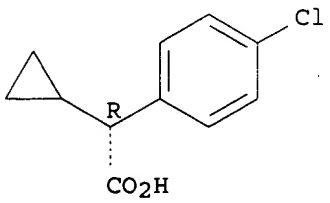
Absolute stereochemistry.



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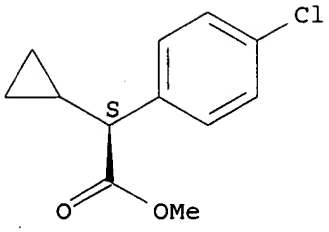

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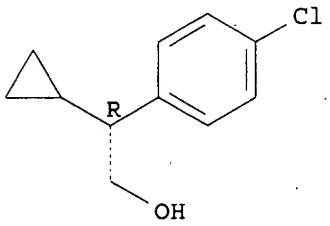
119544-60-4P, (2S)-2-(4-Chlorophenyl)-2-cyclopropylethanol
398453-53-7P, (2R)-2-(4-Chlorophenyl)-2-cyclopropylethyl 4-methylbenzenesulfonate **398453-54-8P**, (2S)-2-(4-Chlorophenyl)-2-cyclopropylethyl 4-methylbenzenesulfonate **398453-55-9P**, (3R)-3-(4-Chlorophenyl)-3-cyclopropylpropanenitrile **398453-56-0P**, (3S)-3-(4-Chlorophenyl)-3-cyclopropylpropanenitrile **398453-57-1P**, (3R)-3-(4-Chlorophenyl)-3-cyclopropylpropanoic acid **398453-58-2P**, (3S)-3-(4-Chlorophenyl)-3-cyclopropylpropanoic acid **398453-59-3P**, Methyl (3R)-3-(4-chlorophenyl)-3-cyclopropylpropanoate **398453-60-6P**, Methyl (3S)-3-(4-chlorophenyl)-3-cyclopropylpropanoate **398453-61-7P**, Methyl (3R)-3-(4-chlorophenyl)-3-cyclopropyl-2-fluoropropanoate **398453-62-8P**, Methyl (3S)-3-(4-chlorophenyl)-3-cyclopropyl-2-fluoropropanoate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; process for prepn. of chiral insecticidal and acaricidal diarylfluorobutenes via enzymic hydrolysis of (4-chlorophenyl)cyclopropylethanoic acid Me ester using esterase)

RN 119544-59-1 HCAPLUS
CN Benzeneethanol, 4-chloro-.beta.-cyclopropyl-, (.beta.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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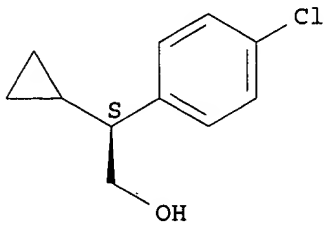
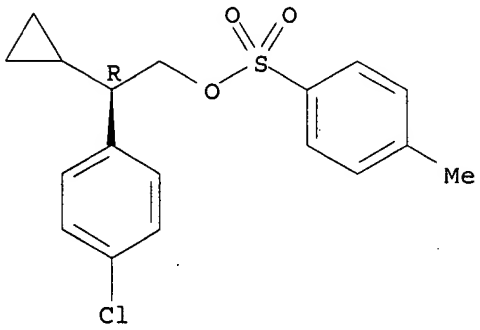
Absolute stereochemistry.



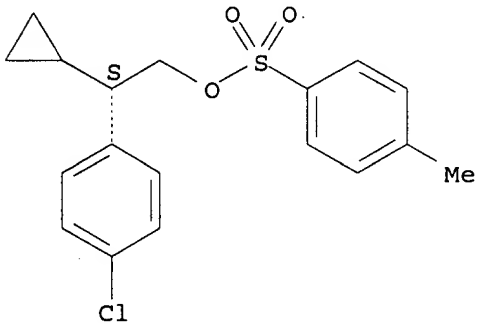
RN 398453-53-7 HCAPLUS
CN Benzeneethanol, 4-chloro-.beta.-cyclopropyl-, 4-methylbenzenesulfonate, (.beta.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



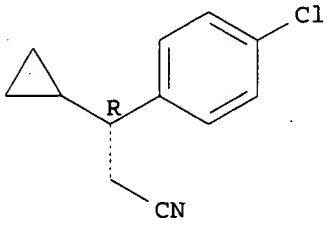
RN 398453-54-8 HCAPLUS
CN Benzeneethanol, 4-chloro-.beta.-cyclopropyl-, 4-methylbenzenesulfonate, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



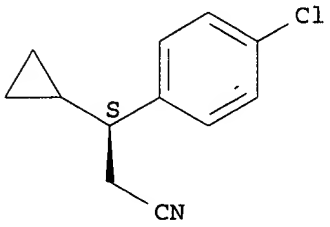
RN 398453-55-9 HCAPLUS
CN Benzenepropanenitrile, 4-chloro-.beta.-cyclopropyl-, (.beta.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



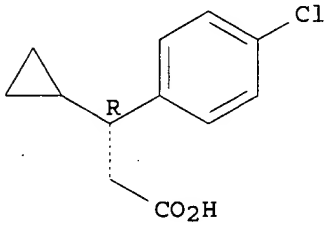
RN 398453-56-0 HCAPLUS
CN Benzenepropanenitrile, 4-chloro-.beta.-cyclopropyl-, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



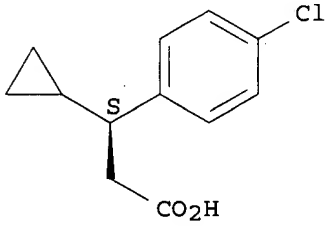
RN 398453-57-1 HCAPLUS
CN Benzenepropanoic acid, 4-chloro-.beta.-cyclopropyl-, (.beta.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



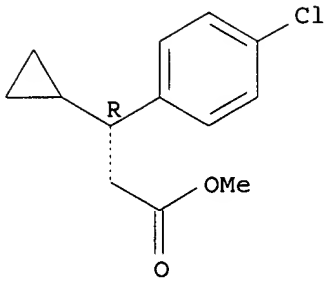
RN 398453-58-2 HCAPLUS
CN Benzenepropanoic acid, 4-chloro-.beta.-cyclopropyl-, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



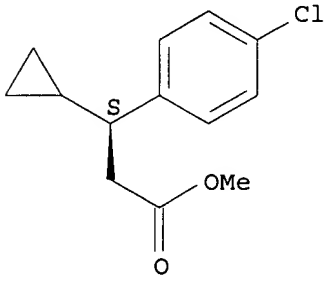
RN 398453-59-3 HCAPLUS
CN Benzenepropanoic acid, 4-chloro-.beta.-cyclopropyl-, methyl ester, (.beta.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



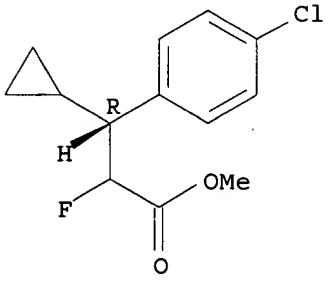
RN 398453-60-6 HCAPLUS
CN Benzenepropanoic acid, 4-chloro-.beta.-cyclopropyl-, methyl ester, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



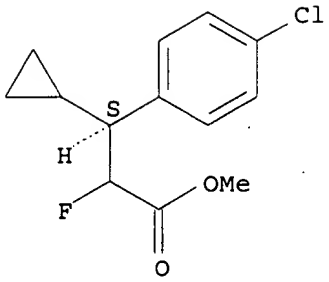
RN 398453-61-7 HCAPLUS
CN Benzenepropanoic acid, 4-chloro-.beta.-cyclopropyl-.alpha.-fluoro-, methyl ester, (.beta.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

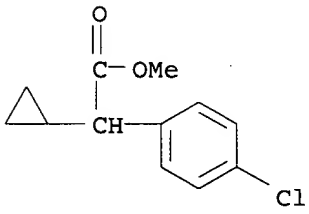


RN 398453-62-8 HCAPLUS
CN Benzenepropanoic acid, 4-chloro-.beta.-cyclopropyl-.alpha.-fluoro-, methyl ester, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **119544-56-8**, Methyl (2RS)-(4-chlorophenyl)(cyclopropyl)ethanoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; process for prepn. of chiral insecticidal and acaricidal diarylfluorobutenes via enzymic hydrolysis of (4-chlorophenyl)cyclopropylethanoic acid Me ester using esterase)
RN 119544-56-8 HCAPLUS
CN Benzeneacetic acid, 4-chloro-.alpha.-cyclopropyl-, methyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:137168 HCAPLUS
DOCUMENT NUMBER: 134:178341
TITLE: Preparation of 2-arylvinyl alkyl ethers and 1,4-diaryl-2-fluoro-2-butenes.
INVENTOR(S): Hu, Yulin; Hunt, David Allen; Liu, Weiguo
PATENT ASSIGNEE(S): American Cyanamid Company, USA
SOURCE: PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001012578	A1	20010222	WO 2000-US21464	20000807

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 6291721	B1	20010918	US 1999-373262	19990812
BR 2000013100	A	20020430	BR 2000-13100	20000807
EP 1202948	A1	20020508	EP 2000-952575	20000807
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003507355	T2	20030225	JP 2001-516879	20000807

PRIORITY APPLN. INFO.: US 1999-373262 A 19990812
WO 2000-US21464 W 20000807

OTHER SOURCE(S): CASREACT 134:178341; MARPAT 134:178341

AB Ar(R)C:CHOR [R = H, alkyl, haloalkyl, cycloalkyl, halocycloalkyl; R1 = alkyl; Ar = (substituted) Ph, naphthyl, heteroaryl], were prepd. in the absence of phosphonium halides by reaction of ArCHRCHO (variables as above) with R1OH in the presence of acid, or reaction of ArCHRCH(OR1)2 in an aprotic solvent at elevated temp. in the presence of acid. Thus, 1-[1-(p-chlorophenyl)-2,2-dimethoxyethyl]cyclopropane (prepn. given) was refluxed with 4-MeC6H4SO3H in PhMe with distn. of PhMe/MeOH to give 96% 1-[1-(p-chlorophenyl)-2-methoxyvinyl]cyclopropane. This in H2O contg. KOH and 18-crown-6 at 7-10.degree. was treated with CHCl2F followed by stirring for 36 h at 10-13.degree., addn. of H2O, and heating at 70-75.degree. for 4 h to give (Z)- and (E)-p-chloro-.beta.-cyclopropyl-.alpha.-fluorocinnamaldehyde as a separable mixt. This was used to prep. (Z)-1-[1-(p-chlorophenyl)-2-fluoro-4-(4-fluoro-3-phenoxyphenyl)-2-butenyl]cyclopropane.

IC ICM C07C041-01
ICS C07C041-28; C07C043-176; C07C043-215; C07C043-29

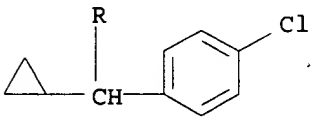
CC 25-9 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

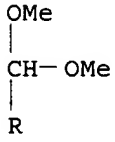
IT 89765-32-2P 89765-34-4P 233760-27-5P 233760-28-6P 269398-38-1P 270080-62-1P 270080-63-2P 270080-64-3P **326801-48-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of 2-arylvinyl alkyl ethers and 1,4-diaryl-2-fluoro-2-butenes)

IT **326801-48-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of 2-arylvinyl alkyl ethers and 1,4-diaryl-2-fluoro-2-butenes)

RN 326801-48-3 HCAPLUS

CN Benzene, 1-chloro-4-(1-cyclopropyl-2,2-dimethoxyethyl)- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:349898 HCAPLUS
DOCUMENT NUMBER: 122:125901

TITLE: Novel 1-cyclopropyl-1-(4-substituted phenyl)-4-cyano-(4-fluoro-3-phenoxyphenyl)butane insecticides

AUTHOR(S): Cullen, Thomas G.; Sieburth, Scott M.; Dybas, Jane A.; Walsh, Michael A.; Meier, Gary A.; Engel John F.

CORPORATE SOURCE: Agric. Chem. Group, FMC Corp., Princeton, NJ, 08543-0008, USA

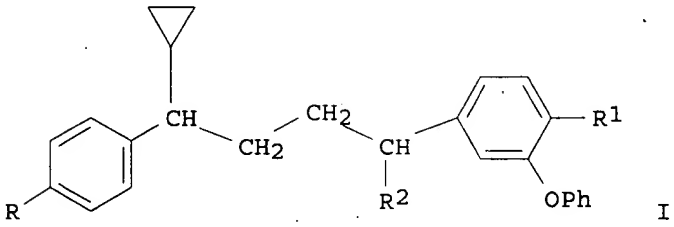
SOURCE: ACS Symposium Series (1995), 584(Synthesis and Chemistry of Agrochemicals IV), 245-54
CODEN: ACSMC8; ISSN: 0097-6156

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB 4-Cyano-1-cyclopropyl-1,4-diarylbutanes (I, R = H, Cl CF3, OCF3, OEt; R1 = H, f; R2 = H, CN, Me) are potent broad-spectrum insecticides, and, in some cases acaricides. The chem. and biol. activity of I are discussed. The biol. activity is compared to both relevant com. stds. and the corresponding unsubstituted compds., the 1,4-diaryl-4-cyclopropylbutanes.

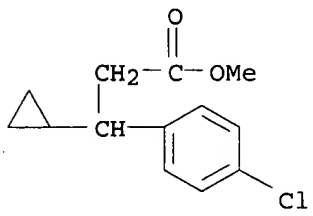
CC 5-4 (Agrochemical Bioregulators)

IT 6640-25-1P 119544-46-6P **147379-48-4P** 147379-49-5P
147379-50-8P 147379-53-1P 147379-67-7P 161042-50-8P 161042-51-9P
161042-52-0P 161042-53-1P 161042-54-2P 161042-55-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(cyclopropyl(substituted phenyl)cyano(fluorophenoxyphenyl)butane insecticides)

IT **147379-48-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(cyclopropyl(substituted phenyl)cyano(fluorophenoxyphenyl)butane insecticides)

RN 147379-48-4 HCAPLUS

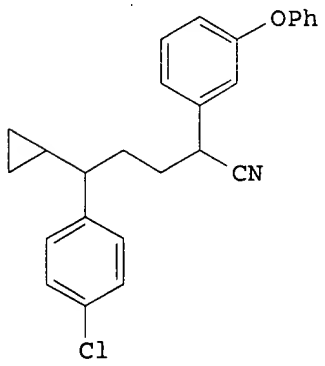
CN Benzenepropanoic acid, 4-chloro-.beta.-cyclopropyl-, methyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1993:233684 HCAPLUS
DOCUMENT NUMBER: 118:233684
TITLE: diaryl(cyclopropyl)pentanenitriles and diaryl(cyclopropyl)butanes and their use as insecticides and acaricides
INVENTOR(S): Cullen, Thomas Gerard; Sieburth, Scott McNeill; Meier, Gary Allen; Engel, John Francis
PATENT ASSIGNEE(S): FMC Corp., USA
SOURCE: PCT Int. Appl., 44 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9301715	A1	19930204	WO 1992-US5049	19920617
W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MG, MW, NO, PL, RO, RU, SD				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
US 5223536	A	19930629	US 1991-734421	19910723
AU 9222581	A1	19930223	AU 1992-22581	19920617

PRIORITY APPLN. INFO.: US 1991-734421 19910723
WO 1992-US5049 19920617
OTHER SOURCE(S): CASREACT 118:233684; MARPAT 118:233684
GI



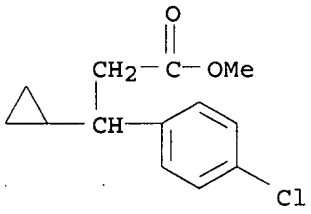
I

AB Some 1,4-diaryl-2-cyclopropylbutane derivs. are claimed. Acaricidal and insecticidal compns. are claimed that contain said compds. Condensation of 3-cyclopropyl-3-(4-chlorophenyl)propanal with 3-phenoxbenzeneacetonitrile gave 1-cyclopropyl-1-(4-chlorophenyl)-4-cyano--4-(4-phenoxyphenyl)-3-butene. Redn. of the latter gave 5-(4-chlorphenyl)-5-cyclopropyl)-1-(3-phenoxyphenyl)pentanenitrile (I). I had foliar insecticidal and acaricidal activity.
IC ICM A01N031-14
ICS A01N037-34; C07C043-263; C07C255-31
CC 25-20 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 5
IT 329-15-7P 62587-07-9P, Cyclopropyl 4-(trifluoromethyl)phenyl ketone

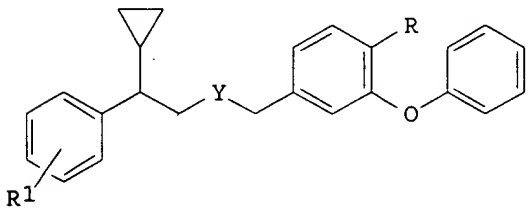
68359-53-5P, 4-Fluoro-3-phenoxybenzenemethanol 75210-42-3P, 4-Fluoro-3-phenoxyphenylmethyl chloride 116332-61-7P, N-Methoxy-N-methyl-4-(trifluoromethyl)benzamide 133333-78-5P, Cyclopropyl 4-(trifluoromethoxy)phenyl ketone 147379-47-3P, Methyl 3-cyclopropyl-3-(4-chlorophenyl)-2-propenoate **147379-48-4P**, Methyl 3-cyclopropyl-3-(4-chlorophenyl)propanoate 147379-49-5P, 3-Cyclopropyl-3-(4-chlorophenyl)-1-propanol 147379-50-8P, 3-Cyclopropyl-3-(4-chlorophenyl)propanal 147379-51-9P 147379-53-1P, 4-Fluoro-3-phenoxybenzeneacetonitrile 147379-54-2P 147379-55-3P 147379-56-4P 147379-57-5P 147379-58-6P 147379-60-0P 147379-61-1P 147379-62-2P 147379-63-3P 147379-64-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for diaryl(cyclopropyl)pentanenitrile (acaricide and insecticide))

IT **147379-48-4P**, Methyl 3-cyclopropyl-3-(4-chlorophenyl)propanoate
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for diaryl(cyclopropyl)pentanenitrile (acaricide and insecticide))

RN 147379-48-4 HCAPLUS
CN Benzenepropanoic acid, 4-chloro-.beta.-cyclopropyl-, methyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1993:34387 HCAPLUS
DOCUMENT NUMBER: 118:34387
TITLE: Highly efficacious non-ester pyrethroid insecticides with low toxicity to fish
AUTHOR(S): Meier, Gary A.; Cullen, Thomas G.; Sehgel, Saroj; Engel, John F.; Burkart, Susan E.; Sieburth, Scott M.; Langevine, Charles M.
CORPORATE SOURCE: Agric. Chem. Group, FMC Corp., Princeton, NJ, 08543, USA
SOURCE: ACS Symposium Series (1992), 504(Synth. Chem. Agrochem. III), 258-70
CODEN: ACSMC8; ISSN: 0097-6156
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Studies directed towards the discovery of insecticides with improved safety to fish have resulted in the identification of 2-cyclopropyl-2-arylethyl (3-phenoxyaryl)methyl ethers and thioethers (I, R = H,F; R1 = H, halo, alkoxy, alkyl; Y = O, S). I show potent activity as broad-spectrum insecticides and, in some cases, acaricides. In addn., I are generally safe to fish and aquatic invertebrates. The 4-fluoro-3-phenoxybenzyl moiety is the most effective pyrethroid alc. equiv. in this series. The ether analogs are more active against insect pests than the thioethers. Configuration at the mol.'s one chiral center is important; the resolved enantiomers of 2-cyclopropyl-2-(4-chlorophenyl)ethyl (4-fluoro-3-phenoxyphenyl)methyl ether demonstrated that the levorotatory isomer was approx. twice as active as the racemic material. Substitution at the 4-position of the phenethyl Ph ring was most important for biol. activity. I tolerated a variety of substituents in this position; however, introduction of CF3 or CF30 not only boosted I activity against lepidopteran and coleopteran species, but also gave rise to potent activity against mites and aphids.

CC 5-4 (Agrochemical Bioregulators)
Section cross-reference(s): 4, 25

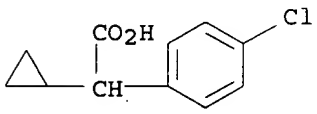
IT **24438-45-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with isopropyloxazolidinone)

IT **119544-59-1P 119544-60-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with methoxytrifluoromethylphenylacetate)

IT **24438-45-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with isopropyloxazolidinone)

RN 24438-45-7 HCAPLUS

CN Benzeneacetic acid, 4-chloro-.alpha.-cyclopropyl- (9CI) (CA INDEX NAME)

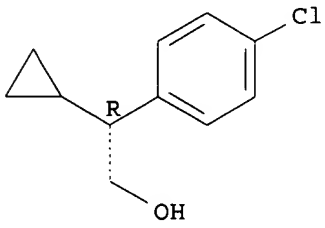


IT **119544-59-1P 119544-60-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with methoxytrifluoromethylphenylacetate)

RN 119544-59-1 HCAPLUS

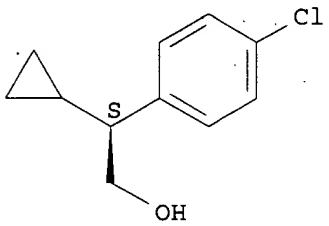
CN Benzeneethanol, 4-chloro-.beta.-cyclopropyl-, (.beta.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 119544-60-4 HCAPLUS
CN Benzeneethanol, 4-chloro-.beta.-cyclopropyl-, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1989:134868 HCAPLUS
DOCUMENT NUMBER: 110:134868
TITLE: Insecticidal cyclopropyl-substituted diaryl compounds
INVENTOR(S): Meier, Gary Allen; Sieburth, Scott Mcneill; Cullen, Thomas Gerard; Engel, John Francis
PATENT ASSIGNEE(S): FMC Corp., USA
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

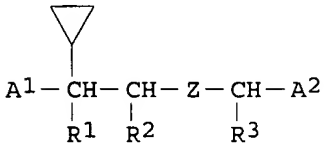
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8808416	A1	19881103	WO 1988-US346	19880205
W: AU, BR, DK, HU, JP, KR, RO, SU				
RW: AT, BE, BJ, CF, CG, CH, CM, DE, FR, GA, GB, IT, ML, MR, NL, SN, TD, TG				
US 4808762	A	19890228	US 1987-94617	19870909
AU 8813457	A1	19881202	AU 1988-13457	19880205
AU 607975	B2	19910321		
EP 357610	A1	19900314	EP 1988-902034	19880205
EP 357610	B1	19920916		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL				
BR 8807472	A	19900327	BR 1988-7472	19880205
JP 02501387	T2	19900517	JP 1988-501923	19880205
JP 06008256	B4	19940202		
HU 52025	A2	19900628	HU 1988-1669	19880205
HU 206074	B	19920828		
AT 80604	E	19921015	AT 1988-902034	19880205
RO 108522	B1	19940630	RO 1988-142108	19880205
CA 1315282	A1	19930330	CA 1988-559970	19880226
CN 88101892	A	19881102	CN 1988-101892	19880330
CN 1020091	B	19930317		
ES 2006406	A6	19890416	ES 1988-1128	19880413
ES 2009260	A6	19890916	ES 1988-1129	19880413
ES 2009597	A6	19891001	ES 1988-1125	19880413
IL 86060	A1	19930114	IL 1988-86060	19880413
PL 153027	B1	19910228	PL 1988-271962	19880421
PL 153033	B1	19910228	PL 1988-277612	19880421

PL 153034	B1	19910228	PL 1988-277613	19880421
ZA 8802879	A	19881228	ZA 1988-2879	19880422
DD 282608	A5	19900919	DD 1988-315008	19880422
DK 8905215	A	19891218	DK 1989-5215	19891020
RU 2002414	C1	19931115	RU 1989-4742289	19891020
CN 1069168	A	19930224	CN 1992-109233	19920804
CN 1041268	B	19981223		
CN 1069962	A	19930317	CN 1992-109234	19920804
CN 1029123	B	19950628		

PRIORITY APPLN. INFO.: US 1987-41551 A 19870423
US 1987-94617 A 19870909
EP 1988-902034 A 19880205
WO 1988-US346 A 19880205
CN 1988-101892 A 19880330

OTHER SOURCE(S): CASREACT 110:134868; MARPAT 110:134868

GI



I

AB Title insecticidal compds. [I; A1 = (substituted) Ph, thienyl; A2 = (substituted) PhOC6H4, 2-methyl-(1,1'-biphenyl)-3-yl, 6-phenoxy-2-pyridyl; R1-R3 = H then Z = O, S, CH2; R1R2 = bond then ZCHR3 = CH2CH2, CH:CH] (II) are prepd. A stirred suspension of NaH in Me2SO was heated 90 min at 80.degree., the resultant soln. was stirred with addn. of 20.8 g MePPh3Br and then Me2SO at ambient temp. for 30 min and at 60.degree. for addnl. 30 min, the reaction mixt. was successively dropwise added at room temp. with 10.2 g cyclopropyl (4-chlorophenyl) ketone and then Me2SO, and the resultant reaction mixt. was stirred 18 h at room temp. to give 8.2 g 1-cyclopropyl-1-(4-chlorophenyl)ethene (III). After an addn. of 0.68M bis(3-methyl-2-butyl)borane in THF to a stirred soln. of 3.5 g III in THF at 0.degree., the resultant mixt. was stirred 1.3 h at 0.degree., 2.5 h at room temp., and 0.75 h at 60.degree., and the latter mixt. was added at 0.degree. with MeOH, aq. NaOH, and 30% aq. H2O2 followed by stirring 18 h at room temp. and then 30 min at 60.degree. to give 3.8 g 2-cyclopropyl-2-(4-chlorophenyl)-ethanol (IV). To a soln. of 0.1 g NaH in THF at 0.degree. was slowly added 0.8 g IV in THF, the resultant mixt. was stirred 30 min at room temp. and then 1.5 h at 55.degree., the reaction mixt. at room temp. was added slowly with 3,4-(PhO)FC6H3CH2Cl in THF followed by stirring 20 h at room temp. and 30 min at 60.degree. to give 0.65 g Et ether deriv. II [R1 - R3 = H, Z = O, A1 = 4-ClC6H4, A2 = 3,4-(PhO)FC6H3] which showed complete control (in 48 h) of beet armyworm and cabbage looper at 100 ppm and also twospotted spider mite, southern armyworm, and Mexican bean beetle at 1000 ppm sprayed on living leaves (their habitation).

IC ICM C07C043-29
ICS C07C043-257; C07C043-20; C07C043-168; C07C043-174; C07C149-273; C07D213-64; C07D317-46; C07D307-78; C07D333-16; A01N031-00; A01N043-06; A01N043-30; A01N043-40

CC 25-1 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 5

IT **24438-45-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

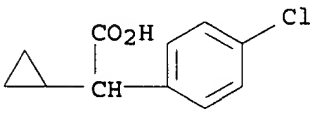
(prepn. and amidation of, with methylethyloxazolidinone)

IT **119544-59-1P 119544-60-4P 119544-80-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and etherification of, with (fluorophenoxyphenyl)methyl chloride)

IT 116332-61-7P 119544-53-5P **119544-56-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrolysis of)

IT **24438-45-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and amidation of, with methylethyloxazolidinone)

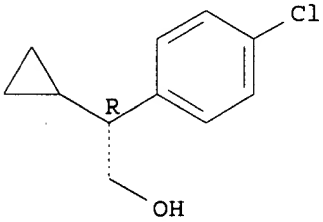
RN 24438-45-7 HCAPLUS
CN Benzeneacetic acid, 4-chloro-.alpha.-cyclopropyl- (9CI) (CA INDEX NAME)



IT **119544-59-1P 119544-60-4P 119544-80-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and etherification of, with (fluorophenoxyphenyl)methyl chloride)

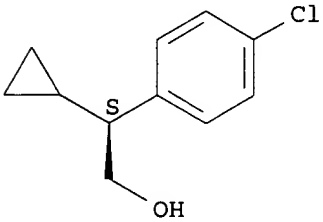
RN 119544-59-1 HCAPLUS
CN Benzeneethanol, 4-chloro-.beta.-cyclopropyl-, (.beta.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

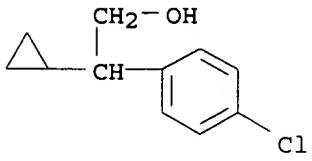


RN 119544-60-4 HCAPLUS
CN Benzeneethanol, 4-chloro-.beta.-cyclopropyl-, (.beta.S)- (9CI) (CA INDEX NAME)

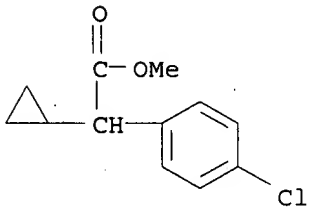
Absolute stereochemistry.



RN 119544-80-8 HCAPLUS
CN Benzeneethanol, 4-chloro-.beta.-cyclopropyl- (9CI) (CA INDEX NAME)



IT **119544-56-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrolysis of)
RN 119544-56-8 HCAPLUS
CN Benzeneacetic acid, 4-chloro-.alpha.-cyclopropyl-, methyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1987:407196 HCAPLUS
DOCUMENT NUMBER: 107:7196
TITLE: Preparation of fungicidal azole derivatives
INVENTOR(S): Grassberger, Maximilian; Schaub, Fritz
PATENT ASSIGNEE(S): Sandoz-Patent-G.m.b.H., Fed. Rep. Ger.
SOURCE: Ger. Offen., 19 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3617190	A1	19861127	DE 1986-3617190	19860522
NL 8601189	A	19861216	NL 1986-1189	19860512
GB 2175899	A1	19861210	GB 1986-12161	19860519
DK 8602376	A	19861124	DK 1986-2376	19860521
SE 8602309	A	19861124	SE 1986-2309	19860521
FI 8602123	A	19861124	FI 1986-2123	19860521
AU 8657653	A1	19861127	AU 1986-57653	19860521
ES 555201	A1	19870716	ES 1986-555201	19860521
BE 904802	A1	19861124	BE 1986-11494	19860522
JP 61271280	A2	19861201	JP 1986-118985	19860522
FR 2582305	A1	19861128	FR 1986-7366	19860523
ZA 8603872	A	19880127	ZA 1986-3872	19860523

PRIORITY APPLN. INFO.: CH 1985-2204 19850523
DE 1986-3606149 19860226

GI For diagram(s), see printed CA Issue.

AB Azoles I [R1, R2 = H, NO2, halo, alkyl, haloalkyl, alkylthio, etc.; R3 = (un)substituted alkyl, alkenyl, alkynyl, Ph, etc.; X = N, CH; n = 2-5] and I salts are prepd. as medical and agricultural fungicides. Thus, a suspension of trimethylsulfoxonium iodide and NaI in abs. DMF was treated with 1,2,4-triazole and 4-chlorophenyl 1-methylthiocyclopropyl ketone (prepn. given) to give .alpha.-(4-chlorophenyl)-.alpha.-(1-methylthio)cyclopropyl-1H-1,2,4-triazole-1-ethanol. Oral administration of I (specific compd. not disclosed) at 0.1-10 mg/kg twice daily controlled intravaginal Candida albicans infection, in the rat.

IC ICM C07D249-08
ICS C07D233-60; A01N043-50; A01N043-653; A61K031-41

ICI C07D249-08, C07D295-04; C07D233-60, C07D295-04

CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 5

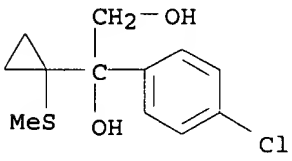
IT 108209-96-7P **108210-03-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and optical resoln. of)

IT **108209-97-8P 108209-98-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with Me chloride)

IT **108210-03-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and optical resoln. of)

RN 108210-03-3 HCAPLUS

CN 1,2-Ethanediol, 1-(4-chlorophenyl)-1-[1-(methylthio)cyclopropyl]- (9CI) (CA INDEX NAME)

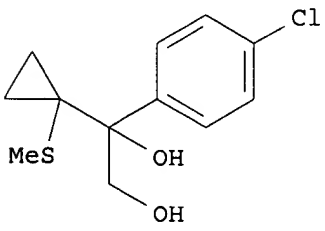


IT **108209-97-8P 108209-98-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with Me chloride)

RN 108209-97-8 HCAPLUS

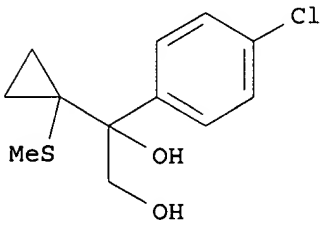
CN 1,2-Ethanediol, 1-(4-chlorophenyl)-1-[1-(methylthio)cyclopropyl]-, (+)- (9CI) (CA INDEX NAME)

Rotation (+).

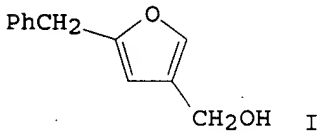


RN 108209-98-9 HCAPLUS
CN 1,2-Ethanediol, 1-(4-chlorophenyl)-1-[1-(methylthio)cyclopropyl]-, (-)-
(9CI) (CA INDEX NAME)

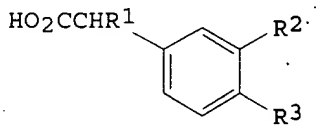
Rotation (-).



L5 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1981:208489 HCAPLUS
DOCUMENT NUMBER: 94:208489
TITLE: The pyrethrins and related compounds. Part XXIV. Synthesis, carbon-13 nuclear magnetic resonance spectra and insecticidal activity of cycloalkyl analogs of fenvalerate
AUTHOR(S): Elliott, Michael; Farnham, Andrew W.; Janes, Norman F.; Johnson, Diana M.; Pulman, David A.
CORPORATE SOURCE: Dep. Insectic. Fungic., Rothamsted Exp. Stn., Harpenden, AL5 2JQ, UK
SOURCE: Pesticide Science (1980), 11(5), 513-25
CODEN: PSSCBG; ISSN: 0031-613X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



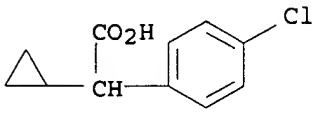
I



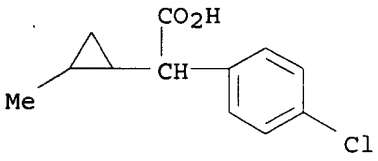
II

AB Forty-two esters of the alcs. 3-PhOC6H4R [R = CH2OH, CH(OH)CN] or I with the acids II (R1 = CHMe2, cycloalkyl, R2, R3 = H, halo, Me, Et) were prepd. and their insecticidal activity against Musca domestica and Phaedon cochleariae was examd. The compds. were relatively nontoxic to mammals, many having LD50 values (i.v.) >400 mg/kg in rats.
CC 25-18 (Noncondensed Aromatic Compounds)
Section cross-reference(s): 5
IT 24438-44-6P **24438-45-7P** 24438-46-8P 34543-12-9P
65363-25-9P 74519-74-7P 76618-96-7P 77585-19-4P 77585-44-5P
77585-46-7P 77585-49-0P **77585-50-3P** 77585-51-4P
77585-53-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and esterification of)
IT **24438-45-7P 77585-50-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and esterification of)
RN 24438-45-7 HCAPLUS
CN Benzeneacetic acid, 4-chloro-.alpha.-cyclopropyl- (9CI) (CA INDEX NAME)



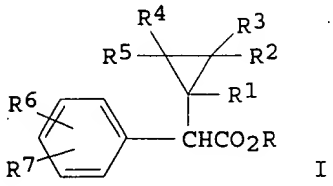
RN 77585-50-3 HCAPLUS
CN Benzeneacetic acid, 4-chloro-.alpha.-(2-methylcyclopropyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1981:103375 HCAPLUS
DOCUMENT NUMBER: 94:103375
TITLE: Carboxylate esters, and pesticide and acaricide compositions
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 55100338	A2	19800731	JP 1979-6716	19790123

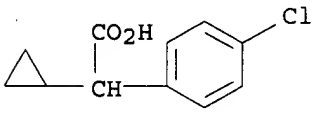
PRIORITY APPLN. INFO.: JP 1979-6716 19790123
GI



I

AB New carboxylate esters contg. heterocyclic moieties (I; R = thienyl, pyrrolyl, imidazolyl; R1-5 = H, Me; R6,7 = H, halo, alkyl, alkoxy, CN, or R6R7 = OCH2O) are prepd. by esterification of the acid of I or its reactive deriv. with RX (X = OH, halo, arylsulfonyl). I had LC50 of 76-260 mg/mL against houseflies.

IC C07C069-013; A01N037-10; A01N043-10; A01N043-30
CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5
IT **24438-45-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thienyl chloride)
IT **24438-45-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thienyl chloride)
RN 24438-45-7 HCAPLUS
CN Benzeneacetic acid, 4-chloro-.alpha.-cyclopropyl- (9CI) (CA INDEX NAME)

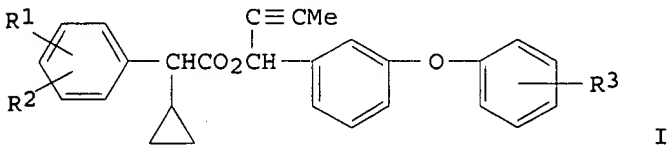


L5 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1980:495015 HCAPLUS
DOCUMENT NUMBER: 93:95015
TITLE: .alpha.-Phenyl-.alpha.-cyclopropyl acetates with pesticidal action
INVENTOR(S): Farooq, Saleem; Ackermann, Peter; Drabek, Jozef; Gsell, Laurenz; Kristianson, Odd; Wehrll, Rudolf
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Eur. Pat. Appl., 19 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 6630	A1	19800109	EP 1979-102186	19790629
R: AT, BE, CH, DE, FR, GB, IT, NL				
JP 55009094	A2	19800122	JP 1979-84369	19790703

PRIORITY APPLN. INFO.: CH 1978-7241 19780703
CH 1979-2560 19790319

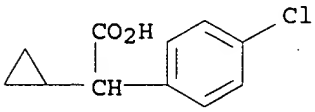
GI



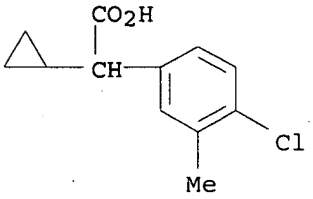
I

AB The title cyclopropylacetates I (R1, R2 = H, halo, C1-4 alkyl; R3 = H, halo, MeO, Me), useful as insecticides, acaricides, and mothproofing agents (no data), were prepd. Thus, refluxing cyclopropyl(4-chlorophenyl)acetic acid in hexane with SOCl2 2 h gave the corresponding acid chloride, which was stirred 12 h at room temp. with pyridine and 3-MeC.tplbond.CCH(OH)C6H4OPh in PhMe to give I (R1 = 4-Cl, R2 = R3 = H).
IC C07C069-743; A01N053-00; C07C043-20

CC 25-18 (Noncondensed Aromatic Compounds)
Section cross-reference(s): 5
IT **24438-45-7**
RL: PROC (Process)
(conversion of, acid chloride)
IT 5689-18-9 24438-46-8 74519-74-7 74519-75-8 **74519-78-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification with phenoxybenzyl alcs. via acid halide)
IT **24438-45-7**
RL: PROC (Process)
(conversion of, acid chloride)
RN 24438-45-7 HCAPLUS
CN Benzeneacetic acid, 4-chloro-.alpha.-cyclopropyl- (9CI) (CA INDEX NAME)



IT **74519-78-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification with phenoxybenzyl alcs. via acid halide)
RN 74519-78-1 HCAPLUS
CN Benzeneacetic acid, 4-chloro-.alpha.-cyclopropyl-3-methyl- (9CI) (CA INDEX NAME)



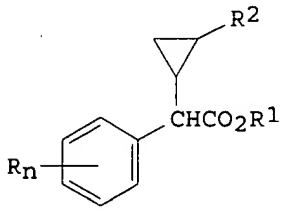
L5 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1978:50521 HCAPLUS
DOCUMENT NUMBER: 88:50521
TITLE: Insecticidal cyclopropylphenylacetic acid esters
INVENTOR(S): Elliott, Michael; Janes, Norman Frank; Pulman, David Allen
PATENT ASSIGNEE(S): National Research Development Corp., UK
SOURCE: Ger. Offen., 26 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2717414	A1	19771103	DE 1977-2717414	19770420
DE 2717414	C2	19871015		
GB 1580193	A	19801126	GB 1976-16234	19760422
NL 7704252	A	19771025	NL 1977-4252	19770419
US 4137324	A	19790130	US 1977-789226	19770420

JP 52131563	A2	19771104	JP 1977-46689	19770421
JP 62029422	B4	19870625		
FR 2348919	A1	19771118	FR 1977-12082	19770421
FR 2348919	B1	19820716		

PRIORITY APPLN. INFO.: GB 1976-16234 19760422

GI



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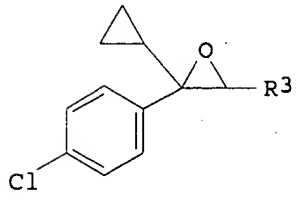


II

AB Twenty-nine insecticidal compds. I (Rn = p-Cl, Br, Me, Et, F, 3,4-Me2, 3,4-CH2O2; R1 = 5-benzyl-3-furyl, 3-PhOC6H4CH2, etc.; R2 = H, Me) were prepd. from I (R1 = H). Thus, p-chlorophenyl cyclopropyl ketone reacted with KOCMe3 and ClCH2CO2Et or with NaH and trimethylsulfoxonium iodide in DMF to give II (R3 = CO2Et) and II (R3 = H), resp., which were hydrolyzed to cyclopropyl(p-chlorophenyl)acetaldehyde. Oxidn. of the aldehyde with AgNO3 gave I (Rn = 4-Cl, R1 = R2 = H), which was converted into insecticidal esters having 1.8-53% of the activity of bioresmethin against houseflies.

IC C07C069-74

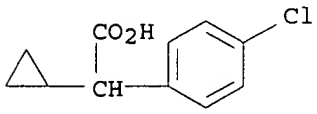
CC 25-18 (Noncondensed Aromatic Compounds)
Section cross-reference(s): 5

IT **24438-45-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and esterification of)

IT **24438-45-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and esterification of)

RN 24438-45-7 HCAPLUS

CN Benzeneacetic acid, 4-chloro-.alpha.-cyclopropyl- (9CI) (CA INDEX NAME)



L5 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:	1970:12378 HCAPLUS
DOCUMENT NUMBER:	72:12378
TITLE:	.alpha.-Phenylcycloaliphatic acids and amides
INVENTOR(S):	Dickel, Daniel F.; De Stevens, George
PATENT ASSIGNEE(S):	CIBA Ltd.
SOURCE:	Ger. Offen., 51 pp. CODEN: GWXXBX
DOCUMENT TYPE:	Patent
LANGUAGE:	German

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1913531	A	19691009	DE 1969-1913531	19690318
NL 6903270	A	19690930	NL 1969-3270	19690303
FR 2004826	A1	19691205	FR 1969-8704	19690325
BE 730523	A	19690926	BE 1969-730523	19690326
US 3786085	A	19740115	US 1969-858893	19690917
US 3880916	A	19750429	US 1973-350447	19730412

PRIORITY APPLN. INFO.: US 1968-716290 19680327
US 1969-789076 19690102
US 1969-808341 19690318
US 1969-858893 19690917

GI For diagram(s), see printed CA Issue.

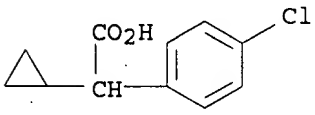
AB The title compds. I and II, which have antiinflammatory properties, were prepd. Thus, a soln. of 18 g tert-BuOK in 130 ml tert-BuOH was added to a soln. of 22.8 g 4-cyclohexylphenyl cyclopropyl ketone and 19.6 g ClCH2CO2Et in 50 ml C6H6 and 20 ml tert-BuOH at 0-5.degree., and the mixt. stirred 25 hrs at room temp. to yield .beta.-(4-cyclohexylphenyl)-.beta.-(cyclopropyl)glycidic acid Et ester, which (36 g) stirred 16 hrs at room temp. with 353 ml EtOH, 1.8 ml H2O, and 39 g KOH gave .alpha.-(4-cyclohexylphenyl)-.alpha.-(cyclopropyl)acetaldehyde (III). A suspension of 33.4 g AgNO3 and 20 g NaOH in 210 ml H2O was treated dropwise with 25 g III in 3 ml EtOH, and the mixt. stirred 16 hrs at room temp. to yield I (R = cyclohexyl, R' = H) (IV), m. 154-6.degree. (hexane); amide m. 151-3.degree.; pyrrolidide m. 137-8.degree.; morpholide m. 115-17.degree.; (-)-1-phenylethylamine (-)-IV salt [.alpha.]25D -27.6.degree. (MeOH); (-)-IV m. 131-41.degree.; (+)-1-phenylethylamine (+)-IV salt [.alpha.]25D 32.1.degree. (EtOH); (+)-IV [.alpha.]25D 60.5.degree. (EtOH). Alternatively, 17.2 g 4-sec-butylphenyl cyclopropyl ketone was added to a suspension of 2.4 g NaH, 22 g trimethylsulfoxonium iodide, and 100 ml Me2SO and the mixt. stirred 1 hr at 50.degree. to give 1-cyclopropyl-1-(4-sec-butylphenyl)ethylene oxide, b0.cntdot.04 81-2.degree., which (5 g) was isomerized in 50 ml C6H6 and 1.64 g BF3.2Et2O to .alpha.-cyclopropyl-.alpha.-(4-secbutylphenyl)acetaldehyde, which in turn was transformed as above into I (R = sec-Bu, R' = H), b0.cntdot.02 60-70.degree.. The following intermediates were also prepd.: .beta.-cyclobutyl-.beta.-(4-fluorophenyl)glycidic acid Et ester, b0.cntdot.07 113-19.degree.; .alpha.-cyclobutyl-.alpha.-(4-fluorophenyl)acetaldehyde, b0.cntdot.07 78-80.degree.; .beta.-(3-chloro-4-cyclohexylphenyl)-.beta.-cyclopropylglycidic acid Et ester, b0.cntdot.01 145-50.degree.; .alpha.-(3-chloro-4-cyclohexylphenyl)-.alpha.-cyclopropylacetaldehyde; 1-(4-cyclohexyl-3-nitrophenyl)-1-cyclopropylethylene oxide; and .alpha.-(4-cyclohexyl-3-nitrophenyl)-.alpha.-cyclopropylacetaldehyde. The following I were prepd. (R, R', and m.p. given): Ph, Cl, 134-6.degree.; Ph, NO2, 135-6.degree.; Ph, H2N, 149-51.degree.; F, H, 61-3.5.degree.; Cl, H, 80-5.degree.; Me, Me, 106-8.degree.; and Ph, H, 97-100.degree.. Also prepd. was II, m. 108-9.5.degree.; amide m. 133-4.degree..

IC C07C; A61K

CC 25 (Noncondensed Aromatic Compounds)

IT 24438-32-2P 24438-33-3P 24438-34-4P 24438-35-5P 24438-36-6P
24438-37-7P 24438-38-8P 24438-39-9P 24438-40-2P 24438-41-3P
24438-42-4P 24438-43-5P 24438-44-6P **24438-45-7P**
24438-46-8P 24438-47-9P 24444-21-1P 24444-22-2P 24444-23-3P
24513-85-7P 24513-86-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **24438-45-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 24438-45-7 HCAPLUS
CN Benzeneacetic acid, 4-chloro-.alpha.-cyclopropyl- (9CI) (CA INDEX NAME)



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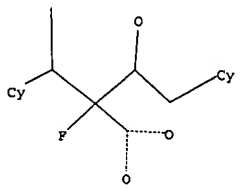

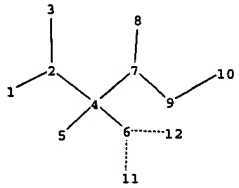

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chain bonds :
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exact/norm bonds :
1-2 6-11 6-12 7-8 9-10
exact bonds :
2-3 2-4 4-5 4-6 4-7 7-9

Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom
11:CLASS 12:CLASS